

23084130 PR-TP-1998-100

MEMORANDUM FOR IN-HOUSE PUBLICATIONS

FROM: PROI (TI) (STINFO)

7 May 98

SUBJECT: Authorization for Release of Technical Information, Control Number: AFRL-PR-ED-TP-1998-100
Talley, Woodward, Kaltz, Long and Micci Experimental and Numerical Studies of Transcritical LOX Droplets"
(Statement A)

ILASS-Europe'98

Manchester 6-8 July 1998

EXPERIMENTAL AND NUMERICAL STUDIES OF TRANSCRITICAL LOX DROPLETS

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ABSTRACT

A 137 atm pressure vessel has been developed for the study of transcritical liquid oxygen and liquid nitrogen droplets and jets. At the same time, numerical modeling of the same phenomena is being pursued using scaled and unscaled molecular dynamics. Experimental and numerical results both show the disappearance of surface tension as the droplet passes through its critical point and the effect of various environment mixtures on the critical point.

INTRODUCTION

Transcritical injection occurs in current high pressure liquid rocket engines where the liquid oxygen is injected into a combustion chamber which is operating above the critical pressure and temperature of the oxygen. The oxygen, initially above its critical pressure, is heated upon injection into the chamber to a value above its critical temperature, thus undergoing a transition from subcritical to supercritical conditions during the atomization and vaporization processes. There are few previous experimental studies of transcritical LOX evaporation due to the difficulty of creating and maintaining liquid oxygen droplets in a high pressure environment. At the same time, CFD studies are hindered by assumptions concerning the solution geometry, equations of state, mixture rules and the need for extensive tables of material properties, some of which change dramatically near the critical point.

EXPERIMENTAL STUDIES

Experimental studies of transcritical oxygen droplets were performed using the droplet generator illustrated in Fig 1. Gaseous oxygen at room temperature was introduced into a central tube at the pressure selected for study (oxygen is actually a supercritical fluid under these conditions). The oxygen was then cooled and densified ("condensed") by a surrounding bath of liquid nitrogen at atmospheric pressure. A piezoelectric crystal (not shown) was mounted in the tube to provide acoustic excitation. Droplets were then formed in the throat of a converging/diverging section surrounded by a flow of gaseous helium (actually also a supercritical fluid) which has also been chilled by liquid nitrogen. The chilled helium served three purposes. First, it helped keep the drop generator tip cold, preventing heat transfer and/or boiling from interfering with drop production. Second, the aerodynamic interaction with the emerging densified oxygen produced a "stripping" action which, in addition to piezoelectric excitation, is also a proven method for producing monodisperse streams of droplets, at least for subcritical flows. The droplets described below were in fact produced using this method; piezoelectric excitation was not used. The third and most important function of the helium was to provide surface tension for forming the droplets. Previous experience showed that it was not possible to create transcritical oxygen droplets in a gas of similar molecular weight such as oxygen or nitrogen, presumably because the reduction in surface tension as the critical pressure was approached did not allow droplets to be formed. Helium is hypothesized to create helium/oxygen mixtures at the interface which have critical mixing pressures much higher than pure oxygen. Thus the interface becomes subcritical and surface tension can exist, even though the pressure is higher than the critical pressure of pure oxygen.

After droplet formation, the helium and droplets flowed into a pressure vessel (13.7 MPa maximum pressure), where the helium formed a buoyant layer at the top and droplets fell into a test gas having controlled composition and at a temperature slightly below room temperature. For safety reasons, nitrogen was used as the test gas in this study. Earlier experience indicated nitrogen/oxygen mixtures exhibited transcritical behavior similar to oxygen/oxygen mixtures. The flows were visualized using backlit shadowgraphy using two 180 degree opposed 133.4 mm sapphire windows. An additional set of oblong quartz windows oriented at 90 degrees to the sapphire windows allows introduction of laser sheets for spontaneous Raman imaging. However, Raman results will not be reported here. Further details concerning the experimental apparatus can be found in (1).

A representative shadowgraph of the results is given in Fig 2. Liquid oxygen droplets having an initial temperature of 177 K were produced in a chilled helium co-flow of about the same temperature and fell into a pure GN_2 gas at a pressure of 6.6 MPa and a temperature of 290 K. The increasing panel numbers in Fig 2 correspond to increasing distances downstream. The 0.254 mm wire visible in panel 1 was inserted as a size reference and also to provide an indication of the degree of optical distortion. Panel 1, which exhibited very low distortion, provides a good indication of the shape of the reference wire, which was not straight. The dark shadows visible in the images are 1.6 mm thermocouples. The buoyant helium layer formed at the top of the pressure vessel extends just below the bottom of panel 1. The fluids seen in panels 2-4 are largely nitrogen and oxygen. A slow nitrogen "wind" is

flowing from right to left in these images. Thus the smooth gray areas to the right of the panels are nitrogen and the lighter colored turbulent areas to the left are in the droplets' wake and are nitrogen/oxygen mixtures.

Quantitative results have not yet been obtained, but qualitatively it was observed that the droplets exhibited no resistance to deformation and therefore no evidence of surfacetension once they dropped below the helium layer. An inverse bag shape can be seen in panel 2, and in panel 4 such shapes are seen to be joined by "tails" in a mushroom shape which is often observed. Globbs of fluid break off at unpredictable times and sizes which spread, contributing to the mixing. Cellular structures can be observed in panel 3, but it is unclear whether this is due to an instability or simply a response to turbulence. Further efforts are underway to quantify these effects as a function of various parameters. Fig 3 shows realizations of the same flow at the same distance downstream as panel 3, but at different times, to provide an indication of the degree of variability in the flow.

NUMERICAL STUDIES

Molecular dynamics (MD) is being applied to modeling supercritical fluid behavior because it eliminates all the assumptions used in CFD by solving for the motions of individual atoms or molecules caused by forces generated by intermolecular potentials. The potential used is a common pair-wise additive potential called the Lennard-Jones 12-6 potential

$$u_{ij}(r_{ij}) = 4\epsilon \left[\left(\frac{\sigma}{r_{ij}} \right)^{12} - \left(\frac{\sigma}{r_{ij}} \right)^6 \right] \quad [1]$$

where u_{ij} is the potential between two atoms i and j and r_{ij} is the interatomic distance. The force between two atoms is the spatial derivative of the potential. The forces on each atom or molecule are summed and Newton's Law is solved for the particle motion. Due to the large number of particles and forces to be summed, parallel processing is used. Results were obtained on 8 to 32 nodes of an IBM SP-2 using MPI. Because the interatomic force is not a long range force and quickly goes to zero as the interatomic spacing increases, only forces on nearby neighbors needed to be calculated, reducing the computation time. Particle decomposition was used to parallelize the problem and periodic boundary conditions were used.

Submicron Droplet Evaporation

MD has been used to simulate three-dimensional subcritical and supercritical evaporation of a submicron droplet using up to 45,000 molecules. The simulation is conducted by first bringing to equilibrium a droplet surrounded by its vapor at 100 K and a gaseous environment at a specified pressure and temperature. At zero time the droplet is placed into the gas with overlapped gas molecules being removed. The gas temperature is maintained at the specified value by heating the gas molecules at the boundaries of the simulation domain. Oxygen and other diatomic molecules are modeled using two atomic Lennard-Jones sites constrained a fixed distance apart. During the evaporation process oxygen molecules leave the droplet and go into the gas. By monitoring the number of molecules in the droplet as the simulation progresses the evaporation rate can be calculated. Liquid oxygen has been modeled evaporating into gaseous oxygen, helium and hydrogen at gas temperatures up to 300 K and gas pressures up to 20 Mpa. For liquid oxygen evaporating into gaseous oxygen, a distinct difference in droplet behavior is observed between subcritical and supercritical environments. Below the critical pressure and temperature of pure oxygen the droplet remains spherical due to surface tension until complete evaporation. Above the critical point surface tension quickly disappears and the droplet becomes convoluted and cloud shaped with segments breaking off before evaporation is complete.

The evaporation of one species into another results in a critical point which is a function of the mixture composition and is often dramatically higher than the critical points of either species. This also has been observed in the MD simulations of liquid oxygen evaporating into gaseous helium or hydrogen. Environment pressures much higher than the critical pressure of oxygen were required to produce the change in droplet behavior described above. A helium pressure of 20 Mpa was not sufficient to produce supercritical evaporation behavior. For hydrogen environments, a pressure of 7.5 Mpa still resulted in subcritical evaporation while a pressure of 20 Mpa did result in the disappearance of surface tension and supercritical evaporation behavior. Figs 4 and 5 show the surface tension force and density at three simulation times for a liquid oxygen droplet vaporizing into a hydrogen environment. Fig 4, with a hydrogen environment at 300 K and 4 Mpa, shows the surface tension and droplet sphericity remaining throughout the evaporation. The disappearance of both surface tension and a spherical droplet geometry for supercritical conditions is evident in Figure 5 where the environment is at 300 K and 20 Mpa.

Micron Droplet Evaporation

In order to model droplet evaporation in convective environments, micron size droplets are needed to prevent the droplets from accelerating to the flow velocity before any significant evaporation can occur. Although previous studies where the number of atoms was varied over one and a half orders of magnitude showed that the simulated evaporation behavior remained the same provided the droplet was in the continuum regime (2), computational capability currently does not permit the simulation of micron size droplets on the atomic level. Two methods for

scaling soft sphere molecules interacting via a Lennard-Jones 12-6 potential are being examined. The first method, proposed by Greenspan (3), matches total system mass and energy. Thus particle mass and the Lennard-Jones parameters ϵ and σ are scaled, respectively, by

$$m_s = \frac{N}{N_s} m \quad \epsilon_s = \frac{N}{N_s} \epsilon \quad \sigma_s = \sqrt[3]{\frac{N}{N_s}} \sigma \quad [2a, b, c]$$

where N is the number of particles and the subscript s denotes the scaled quantities. The second method, proposed by Long and Micci (4), matches a characteristic temperature and density, defined by

$$T^* = \frac{kT}{\epsilon} \quad \rho^* = nm\sigma^3 \quad [3a, b]$$

where the superscript asterisk denotes a characteristic variable. This results in scaling σ by eqn [2c] but keeping ϵ and particle mass constant. Fig 6 compares the two scaling methods to an unscaled simulation of supercritical oxygen droplet evaporation for a scaling factor of 10 to 1. Both methods match the unscaled evaporation rate within the statistical uncertainty resulting from the small scaled system sizes. Fig 7 shows the supercritical evaporation of a micron LOX droplet obtained with the second method and a scaling factor of a million to one. The number of droplet molecules raised to the two thirds power is proportional to the surface area, thus a D^2 versus time evaporation behavior would be a straight line. It can be seen that the droplet follows the D^2 law for a large part of its evaporation.

CONCLUSIONS

An experimental facility has been developed to generate LOX droplets and pass them into a supercritical environment. Experiments have shown the disappearance of the droplet surface tension as it passes through its critical point and the effect of various environment mixtures on the critical point. Molecular dynamics is proving itself as a means of simulating the supercritical behavior of both submicron and micron sized droplets and has reproduced qualitatively the experimentally observed behavior.

REFERENCES

- 1 Woodward RD & Talley DG, *Raman Imaging of Transcritical Cryogenic Propellants*, AIAA Paper 96-0468, Proc 34th Aerospace Sciences Meeting, Reno, NV, USA, Jan. 1996, pub AIAA, Reston, VA.
- 2 Kaltz TL, Long LN, Micci MM & Little JK, *Supercritical Vaporization of Liquid Oxygen Droplets Using Molecular Dynamics*, scheduled for publication in Combustion Science and Technology.
- 3 Greenspan D, *Particle Modeling*, Birkhauser, Boston, 1997.
- 4 Long LN, Micci MM & Wong BC, *Molecular Dynamics Simulations of Droplet Evaporation*, AIAA Paper 94-2907, Proc 30th Joint Propulsion Conference, Indianapolis, IN, USA, June 1994, pub AIAA, Reston VA.

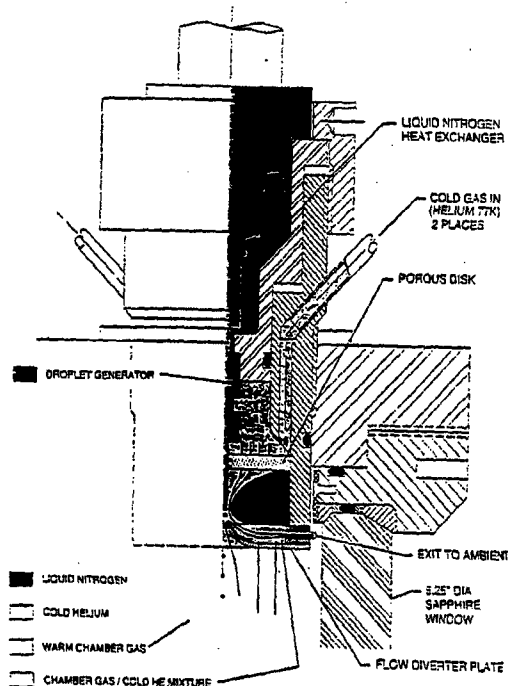


Fig 1. Pressure vessel/droplet generator interface.

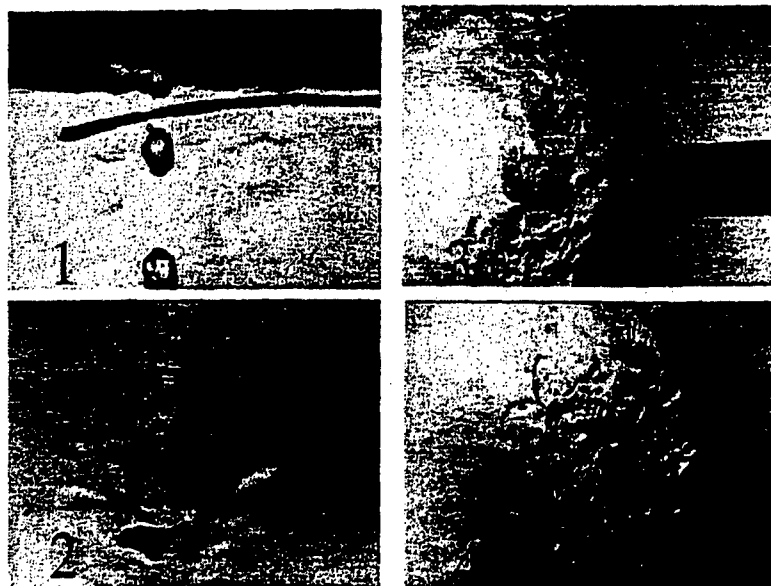


Fig 2. Transcritical LOX droplets falling into GN2. Increasing panel numbers correspond to increasing distances downstream.

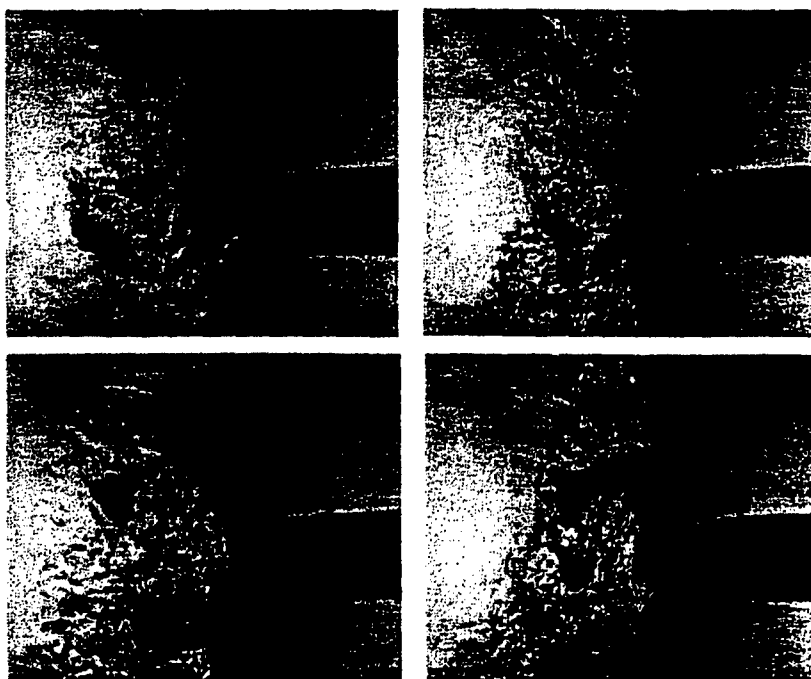


Fig 3. Variability in transcritical droplet stream at the same distance as position 3 in Fig 2.

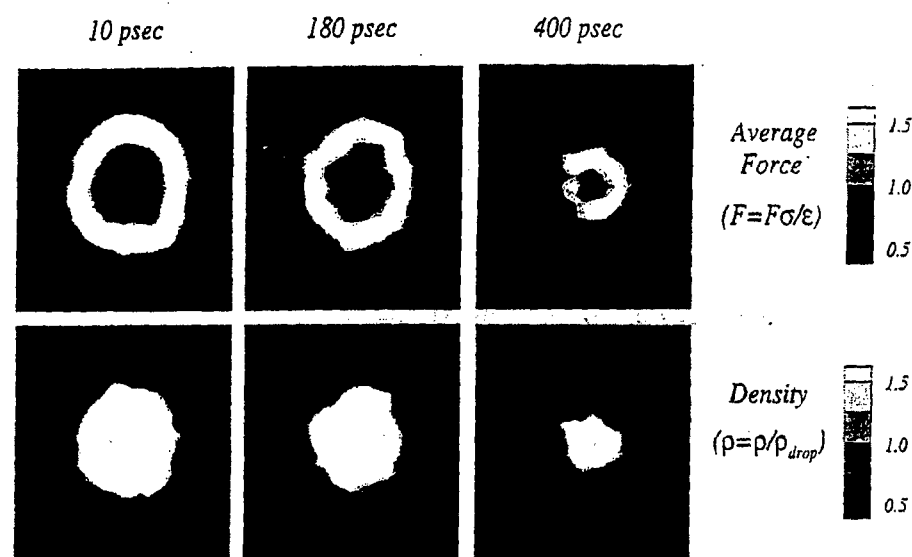


Fig 4. Contour plots of average force and density at 10, 180, and 400 picoseconds of simulation time for a LOX droplet in hydrogen at 300 K and 4 MPa. The average force is an indication of the surface tension experienced by the droplet. The density is non-dimensionalized so the droplet surface density is equal to one.

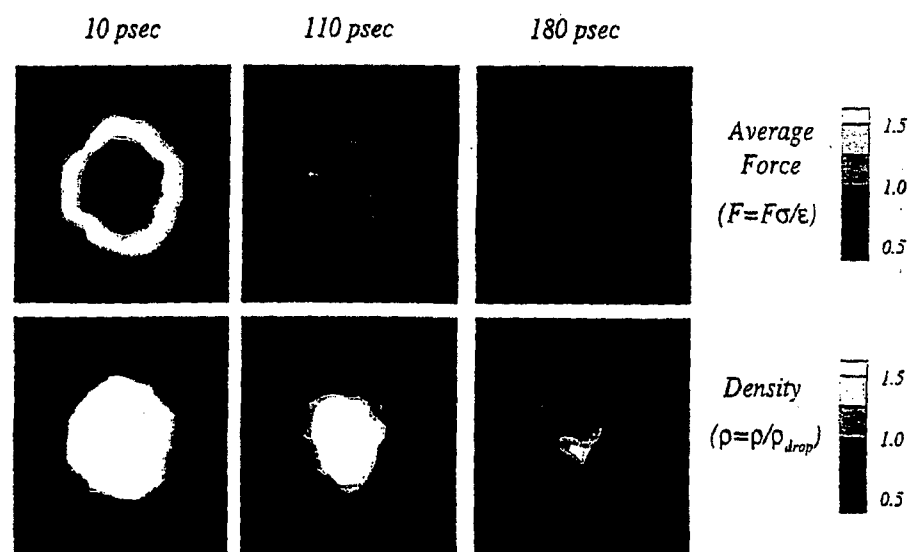


Fig 5. Contour plots of average force and density at 10, 110, and 180 picoseconds of simulation time for a LOX droplet in hydrogen at 300 K and 20 MPa. The average force is an indication of the surface tension experienced by the droplet. The density is non-dimensionalized so the droplet surface density is equal to one.

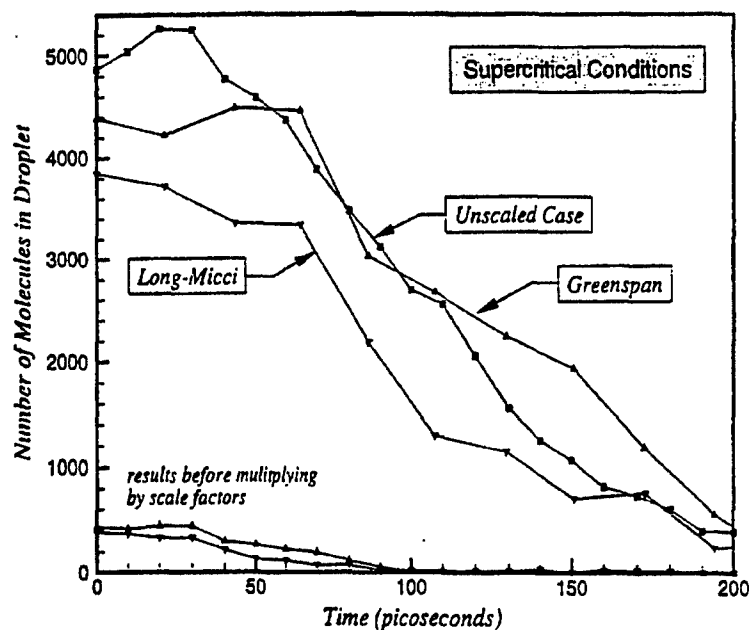


Fig 6. Comparison of evaporation rates between the two scaling methods for a supercritical case. The environment is at 200 K and 12.5 MPa. The ratio of real to scaled particles is 10 to 1.

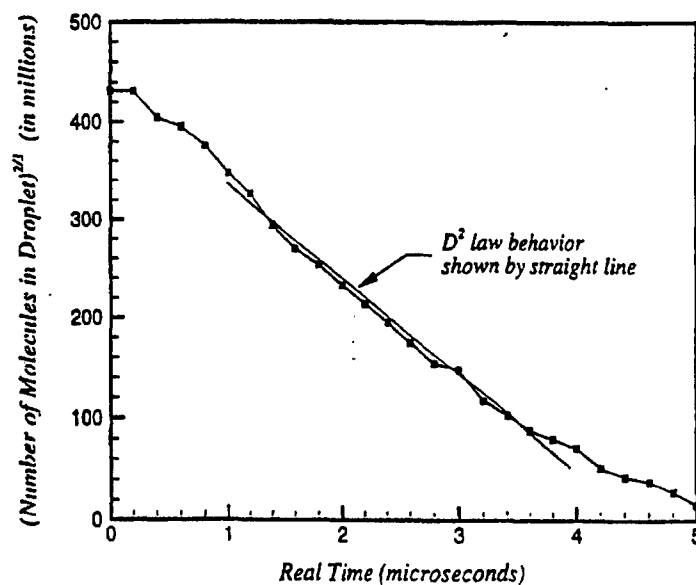


Fig 7. Comparison of micron droplet evaporation rate with D^2 law behavior. The straight line is not the slope predicted from the D^2 law, but is simply to illustrate the portion of the curve to be compared.